TECHNICAL MEMORANDUM

Proposed Modeling for RI/FS
Waukegan Manufactured Gas and Coke Plant Site
July 1, 1991

Prepared for
North Shore Gas Company

Prepared by
Barr Engineering Co.

TECHNICAL MEMORANDUM

PROPOSED MODELING FOR RI/FS

WAUKEGAN MANUFACTURED GAS AND COKE PLANT SITE

JULY 1, 1991

INTRODUCTION

Models of groundwater flow and potential contaminant transport will be used to support the remedial investigation/feasibility study (RI/FS) of the Waukegan Manufactured Gas and Coke Plant (WCP) site. This technical memorandum has been prepared by Barr Engineering Co. for North Shore Gas Company, in accordance with the September 27, 1990 Administrative Order on Consent to describe the objectives of the modeling and present a summary of the anticipated modeling methods.

OBJECTIVES

Based on the anticipated scope of work for the WCP site RI/FS, the objectives of developing models of groundwater flow and potential contaminant transport at the WCP site are:

- to provide interpretive tools for integrating field data and conceptual hydrogeologic models of site conditions, thereby reducing ranges of uncertainty in hydrogeologic parameters;

- to provide an initial evaluation of likely groundwater flow patterns following the first phase of investigations to optimize the locations of monitoring wells to be installed during the second phase;

- to assess potential chemical constituent concentrations at identified or assumed receptor locations for use in assessing environmental and human health risks.

The proposed methods for developing models of groundwater flow and potential contaminant transport are outlined below. If later evaluations of project conditions indicate that different methods are appropriate, these methods will be documented and provided to the U.S. EPA for review.

GROUNDWATER FLOW MODELING

Computer Code

Simulations of groundwater flow will be performed using the Single Layer Analytic Element Model (SLAEM). SLAEM is a commercially available, quasi-three dimensional analytic element code for simulating flow in a single aquifer. A technical summary of the code is included in Attachment A. Detailed discussions of the theoretical derivation of the model are presented in the textbook Groundwater Mechanics by O.D. L. Strack (1989).

Barr has applied the SLAEM code to a variety of groundwater modeling projects, ranging from simple simulations of pumping wells in assumed uniform flow fields to detailed, complex analyses of remedial measures for contaminated groundwater. We have found SLAEM to be significantly more useful than finite-difference or finite-element codes because no grid restrictions or artificial boundaries need be incorporated in the groundwater simulations. Models developed using SLAEM can therefore account for regional influences on local flow systems and can incorporate realistic representations of the locations and shapes of irregular features that influence groundwater flow. In addition, SLAEM avoids difficulties often encountered when using finite-difference or finite-element codes to simulate

individual remedial pumping schemes; these codes generally require finer grid spacing near groundwater withdrawal locations and thus can involve establishing several different grids as various withdrawal schemes are considered. The analytic element method incorporated in SLAEM does not involve a grid and therefore does not limit the consideration of groundwater extraction locations.

SLAEM can simulate steady-state hydrogeologic features such as permeability inhomogeneities, variations in aquifer geometry, fully- and partially-penetrating rivers and lakes, fractures, drains, impermeable walls, leaky walls, variable infiltration, extraction wells, leakage from overlying and underlying aquifers, and stratified aquifer horizons. The code can also simulate the transient effects of wells. Plan view and cross-sectional views of steady-state and transient flow paths can be generated. Capture zones of groundwater extraction systems are evaluated by tracking particle transport in groundwater flow fields computed for the site-specific hydrogeologic system and extraction system design.

Model Set-Up

The configuration of hydrogeologic features to be included in the simulations of groundwater flow at the WCP site will be determined based on information collected during the RI/FS. It is anticipated that the modeling will address two-dimensional horizontal groundwater flow in the near-surface unconsolidated sand unit. The lower boundary of the model will be the underlying gray till unit, and the upper boundary will likely be treated as an unconfined surface within the sand unit. The presence of Lake Michigan/Waukegan Harbor on the east, south, and west sides of the site will be simulated using a series of specified head line sinks. The presence of the new boat slip in the northwestern portion of the site will be similarly incorporated in the modeling. The slurry wall at the east end of the new

slip will be simulated as a leaky wall. Areal recharge values will be assigned as appropriate.

Input Data

Groundwater flow modeling will incorporate estimated values for the following hydrogeologic parameters: (1) hydraulic conductivity; (2) areal recharge; (3) aquifer thickness and/or elevations of the base of the sand aquifer; (4) effective porosity; and (5) surface water elevations in Lake Michigan and Waukegan Harbor. Values for these parameters will be estimated during the RI/FS based on soil investigations, field testing and measurements, and published data. Values for other parameters that may be required (such as elevations of any upper confining layers that may be identified, or specifications for possible groundwater extraction systems) will be determined as necessary.

Simulations

Simulations will be performed to represent observed groundwater flow conditions at the WCP site. Because the new boat slip is now in place (i.e., before groundwater elevation data for the site are available), the simulations of existing conditions for the site will represent flow patterns responding to the influence of groundwater discharge to the new slip. Therefore, simulations will also be performed for conditions prior to the construction of the new slip to assess probable pre-existing flow patterns.

Simulations will be performed using groundwater elevations and slug test data from the first phase of the RI to provide an initial estimate of groundwater flow patterns at the site. The results, coupled with the results of the test trenching source area investigations, will be used to guide placement of groundwater monitoring wells to be installed in the second phase

of the RI. The model will be refined following the collection of additional groundwater elevations, slug test data, and pumping test results during the second phase. Subsequent simulations of potential remedial measures for groundwater will be performed as appropriate during the FS.

SIMULATION OF POTENTIAL CONTAMINANT TRANSPORT

Computer Code

The SLAEM code described above is capable of simulating retardation and biodegradation for solute transport along computed flow paths. Additionally, simulations of solute transport may be performed using the MYGRT Version 2.0 code (EPRI, 1989). MYGRT is a two-dimensional analytical model for simulating the transient migration of organic and inorganic chemicals in groundwater. The code considers advection, dispersion, retardation, and biodegradation, and models can be developed for horizontal (areal) or vertical (cross-sectional) applications. A summary of the theoretical basis of the code is included in Attachment B.

Model Set-Up

The MYGRT code may be used for: (1) areal simulations of contaminant transport in regions of relatively uniform groundwater flow; (2) cross-sectional simulations of contaminant transport along flow paths determined from groundwater elevation data and results of the flow simulations; and (3) one-dimensional simulations of transport along specific flow paths (the SLAEM code may also be used for this application).

Contaminant source areas will likely be simulated as constant concentration sources. Simulations will be performed using compound-specific

data for transport of chemical constituents of interest. Contaminant transport for various remedial alternatives will be evaluated as appropriate.

Input Data

Input data for simulations of contaminant transport will include: (1) groundwater pore velocities; (2) longitudinal and transverse dispersivity values (scale-dependent estimates); (3) compound-specific retardation factors (estimated from octanol/water partition coefficients and aquifer organic carbon content); (4) biodegradation or abiotic decay rates (from published data); and (5) source area groundwater concentrations (based on observed concentrations near source area or on computed concentrations based on soil data and partitioning coefficients).

Simulations

It is anticipated that contaminant transport simulations will be developed to interpret observed groundwater quality data and project potential future concentrations for various remedial scenarios (including the no-action alternative). Simulations will also be performed as appropriate to compute potential groundwater concentrations for identified or assumed receptors for use in the risk assessment. It is likely that the significance of the contaminant transport analyses will be to evaluate the importance of retardation and degradation on transport of polynuclear aromatic hydrocarbons (PAHs) and volatile aromatic compounds.

REFERENCES

Electronic Power Research Institute (EPRI), 1989. MYGRT Code Version 2.0: An IBM Code for Simulating Migration of Organic and Inorganic Chemicals in Groundwater. Prepared by Tetra Tech, Inc., Lafayette, California. Publication EN-6531, Research Project 2879-2.

Strack, O. D. L., 1989. Groundwater Mechanics. Prentice-Hall, Inc., Englewood Cliffs.

Attachment A

Technical Summary

SLAEM
Single Layer Analytic Element Model

A new generation of analytical expressions has recently been developed for a wide range of groundwater hydrologic functions by Dr. Otto D. L. Strack of the University of Minnesota and presented in his book, *Groundwater Mechanics* (Prentice-Hall, 1989). These expressions are implemented in a modular computer model designed for single aquifer modeling, called the Single Layer Analytic Element Model, or **SLAEM**. This model is available for use on personal computers under DOS, and on DSI coprocessor boards.

THEORETICAL BASIS

The analytic element method is a technique for modeling groundwater flow in two and three dimensions. The method is based on the superposition of analytic functions, each representing a particular hydrologic feature of the aquifer or a part thereof. These analytic features are referred to as analytic elements. Each element is selected and inserted into a modeling run to simulate the hydrologic effects of the aquifer feature in question.

Boundary conditions are applied at selected points (called control points) of the boundaries of the aquifer features, giving one equation per control point. The total number of control points is equal to the total number of parameters in the solution. This system of equations is solved for the unknown parameters.

Once all parameters are determined, an approximate analytic solution of the problem is known. Although approximate, the solution is truly analytic. Potentiometric heads can be computed at any point in the aquifer without the need for interpolation, and velocities can be obtained by analytical differentiation. The latter eliminates concerns of numerical dispersion for contaminant transport problems. The derivation of the analytic elements is contained in *Groundwater Mechanics*.

COMPUTER SYSTEMS

SLAEM is available for various configurations, to fit your computer system. The DOS configuration of version 1.1, which runs on a personal computer based either on an Intel 8086, 80286, or 80386 processor, is capable of dealing with 200 equations, which is sufficient for most applications. This configuration is based on the Microsoft compiler. System requirements are: 640K of RAM, a math coprocessor, and graphics capabilities.

To increase the maximum number of elements and enhance computational speed, configurations of SLAEM have been developed that run on 80286 and 80386 based systems. These versions are capable of accessing any amount of available extended memory, are based on the Lahey 16 bit and 32 bit compilers, and require a minimum of 2Mb of extended memory, a mathematics coprocessor, and graphics capability. These configurations of SLAEM are available at an additional cost, which includes a customized configuration to fit your system. SLAEM also runs on DSI-32 series and DSI-780 series coprocessor boards offered by Definicon; these configurations also can acces all memory installed on the boards, and are available at an additional cost.

Graphics support is provided via drivers developed by GSS, which are available for virtually any graphics device available, including CGA, EGA, VGA, and HGA displays, and most plotters and printers.

STRUCTURE

SLAEM was developed using a modular structure with a strong emphasis on interactive graphics. This structure allows the modeler to move quickly and interactively among the modeling tasks involved. These modules are briefly described in the following section. Several versions of SLAEM have been developed so far: version 1.1, version 2.0, and a special version capable of dealing with stratified aquifers, SLAEMS version 2.0.

DESCRIPTION OF ANALYTIC ELEMENTS AND OTHER MODULES (VERSION 1.1)

This section gives an overview of the analytic element modules and of the service and command modules. Many of the options and several examples of their applications are given. Unless otherwise stated, all are steady-state elements. A complete description of the modules and their options is given in the user's manual which is separately available upon request.

- **Aquifer** conditions generally prevailing over the modeled domain: hydraulic conductivity, thickness, base elevation, specific storage, and porosity.
- **Given** elements for which all parameters are known beforehand. These include net infiltration, uniform flow, and circular ponds with a given rate of extraction or leakage.
- **Wells** of three types: with a given discharge, with a given head, or a transient well with a given discharge.
- **Line-sinks** for simulating narrow rivers or creeks and any other boundary with known head. These elements may be specified either with a given head or with a given extraction rate or strength. Strings of line-sinks can be used to approximate the configuration of the streams represented.
- **Area-sinks** are quadrilateral elements with constant extraction from or infiltration to the aquifer through the upper boundary. These may be specified either with a given head and hydraulic resistance or with a given extraction rate or strength. Area-sinks are often used to represent shallow lakes, wetlands, wide rivers, and impervious surfaces.
- **Double root elements** are used for simulating single straight and narrow features such as canal with a given head, drains with a constant but unknown head, cracks, leaky walls, and impermeable walls.
- **Doublet elements** are used to simulate areal inhomogeneities resulting either from differences either in hydraulic conductivity, or in base elevation and/or thickness. Boundaries of inhomogeneities are modeled as straight line-doublets with quadratically varying density distribution and share common boundaries if their nodal points are within a certain specified distance from each other.
- **Grid** and **Plot** modules are used to produce contour plots of head, potential, or streamline distributions; the degree of refinement is adjustable.
- **Section** makes it possible to generate cross-sectional plots.
- **Trace** generates pathlines in three-dimensional space using a Runge-Kutta iterative procedure. The pathlines can be viewed both in plan and in section. This module supports contaminant transport processes such as retardation and decay. The three-dimensional coordinates of the starting point can be entered either manually or graphically using the cross-hair on the plot on the screen.
- **Map** allows a background map of cultural features or observed contours to be generated and plotted.
- **Window** establishes the area over which plotting will occur. This can be changed at any time to allow the modeler to 'step back' from or 'zoom in' on a particular area.
- **Pset** controls the flow of graphics created by SLAEM. It allows textual and numeric data output and graphical output to be displayed on either a two-monitor or a single-monitor system in monochrome or color and for graphics to be generated on the screen, a printer, a plotter, or recorded on a file.
- **Switch** makes it possible to re-direct input and output. Its uses include preparation of several stand-alone and linked input files; direction or echoing of output to monitors, plotters, or printers; and direction or echoing of log files for messages and errors. Typically, this module is used to facilitate input via a string of input files, and to direct calibration data to monitors or printers.
- **Solve** and **Iterate** cause the system of equations to be solved.
- **Check** allows the computed heads and discharges to be examined both for the elements with parameters calculated in the Solve/Iterate module and for those points with head data (e.g. piezometers). This module should be used throughout the model calibration process.
- **Save** and **Read** modules allow solutions to the system of equations to be saved in binary form.

ENHANCEMENTS AVAILABLE IN VERSION 2.0

Version 2.0 of SLAEM is an enhancement of the program described above. The enhancements consist both of improvements that deal with the technical aspects of modeling, and of improvements designed to assist in organizatorial aspects of modeling. Only the most important improvements are listed here.

Technical Aspects

- In addition to the constant-strength line-sinks, line-sinks with linearly varying strength are now available. These elements simulate extraction or infiltration along the line-element as a function that varies linearly. Linear line-sinks are particularly useful when applied in strings; in many cases these elements are nearly twice as efficient as the constant-strength line-sinks.
- Inhomogeneities of hydraulic conductivity can be combined with inhomogeneities in the base elevation and/or thickness.
- The iterative procedure used to model inhomogeneities in base elevation and thickness has now been optimized both for confined and unconfined conditions. The user can choose the optimum procedure to reduce greatly the time required for solving problems in confined systems.
- Area-sinks can be specified both at the bottom and the top of the aquifer. Since these elements can be either resistance specified or strength specified, the single layer program can now be used to model systems of more than one aquifer. Although much less efficient than a multi-aquifer program such as MLAEM, this feature broadens the applicability of SLAEM greatly. Using the sectional feature of trace, streamlines can be produced in section, going from area elements at the top of the aquifer to area elements at the bottom.
- Backward tracing is supported: the user can start a streamline or pathline at any point in the aquifer, at any elevation, and at any time, and the program will track this streamline or pathline backward through time. As for forward streamline tracing, backward tracing is based on analytical expressions for the velocities, so that numerical dispersion is practically zero.
- If a complex problem is to be solved for a number of slightly different cases (e.g. with wells in different positions, or of different discharges) then, once the problem is solved, solutions for the other cases can be obtained, making use of the solution for the first case, by use of the command *reiterate*. If, for example, a solutions would normally require 5 iterations, the slightly modified problem can be solved in one or two steps, resulting in a significant saving of time.
- If conflicting conditions are applied, the program flags it (e.g., two different heads specified at a single point.) If such a condition is flagged, the program will not solve the problem. Note that this applies only to conflicts that make a solution impossible; poorly defined problems are not flagged.
- Data pertaining to transient wells (such as the specific storage coefficient) are now written and read as part of the binary files.

Organizational Aspects

- Prefixes (i.e., directory paths) can be set individually to define the directories input is read from, output is written to, binary files are read from, binary files are written to, and help files are written from. These five prefixes can be set individually and cleared with a single command. The prefixes can be overruled at any time by including the drive letter in the file name.
- Input files can not only be chained but also nested. This makes it possible to create a master input file that calls individual input files, each containing data specific to an area. This is particularly useful for refining certain areas in the model while leaving the rest unchanged.
- Labels can be specified for all of the elements, by entering a label of up to 16 characters between brackets following the element data. These labels are included in any numerical information that the program provides about the element. The labels are intended to make it easier for the modeler to identify the elements other than by their position in the input file.
- Contour plotting is facilitated by adding the capability to produce default contour starting levels and increments.
- Grids can be subtracted, so that draw-down plots can be easily produced by subtracting grids valid for different conditions.

- Grids can be printed in numerical form, either as x, y, z, or in a form that can be read by the computer program SURFER.
- Upon startup, the program will read a file called *initaem.dat*, if it exists. This file can be used to define machine-specific default data the program is to assume (e.g., the number of screens, whether in color or black and white, the default window and hydraulic conductivity).
- There is now a command *reset*, which causes the program to assume all the original default values. Individual *reset* commands are available in all of the analytic element modules, so that, for example, all wells can be removed, without affecting any of the other elements entered.
- When reading an input file, the program automatically echos input to the screen, while suppressing program prompts (messages).

The upgrade to version 2.0 is available separately. This version will be supplied for whatever configuration(s) the user already possesses.

SLAEMS, SLAEM WITH AQUIFER STRATIFICATION.

SLAEMS is a new single layer model, capable of simulating stratification of the aquifer. The theory behind this version of the program is outlined in Section 11 of *Groundwater Mechanics*, and is based on the assumption that the resistance to flow in the vertical direction is negligible with respect to the extent of the aquifer. This assumption (the Dupuit-Forchheimer assumption) implies that the head does not vary in the vertical direction. The strata can be entered (up to a total of 20) globally. In addition, inhomogeneities may be specified which have their own stratification characteristics. Tracing of streamlines is supported, and the refraction of the streamlines at the interfaces of the strata is reproduced in the sectional plots of streamlines.
The strata version is available as an upgrade for users of SLAEM version 2.0. This version will be supplied for whatever configuration(s) the user already possesses. The configuration based on the Microsoft compiler can handle up to 130 equations; the other configurations can handle up to 800 equations for machines with 3 Mb or more of extended memory.

THE PLOTTING PROGRAM PLAEM.

A separate program, PLAEM, is available at additional cost, to enhance the plotting capabilities of all of the analytic element programs. These programs support a command *fiplot*, which allows the user to record on a file everything produced on the screen. The program PLAEM, used preferably on two-monitor systems, can be used to select plots to be produced in hard-copy, and to merge, overlay, or modify each of the individual plots. This program is capable of producing a postscript file, that can be read and manipulated by many other programs. The primary purpose of PLAEM is to let the modeler concentrate on the modeling, and select the appropriate plots later. The format of *fiplot* is an extremely compact binary format, so that a large number of plots can be combined in a single file of manageable size. PLAEM can be used to combine separate files produced via *fiplot* in a new file. Because the *fiplot* files are in binary form, a separately configured executable of PLAEM is required for each configuration of SLAEM: the Microsoft, 286, 386, or DSI configuration. Purchasers of PLAEM will obtain all necessary configurations.

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Attachment B

MYGRT™ Code Version 2.0: An IBM Code for Simulating Migration of Organic and Inorganic Chemicals in Groundwater

EN-6531
Research Project 2879-2

Final Report, October 1989

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Section 4

THEORETICAL BASIS FOR MODEL

THEORY

The MYGRT Code Version 2.0 is a quasi-analytical model based on the advection-dispersion-retardation-decay equation. The processes included for inorganics are advection, dispersion, and linear sorption (retardation). These processes plus net transformation or decay are included for organics. The equations for both one- and two-dimensional cases, their solutions and assumptions are presented in this section.

Governing Equation and Solution for Two-Dimensional Case

Because it is likely to be used more often, the two-dimensional case is discussed first. The partial differential equation with all four of the above processes is given below and in Figure 4-1:

$$R_d \frac{\partial c}{\partial t} + V_x \frac{\partial c}{\partial x} = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} - kcR_d \qquad (4\text{-}1)$$

where

R_d = retardation factor for linear, equilibrium sorption (dimensionless), if no sorption ($R_d = 1$)

c = concentration of solute in groundwater (mg/l or μg/l)

t = time (yr)

V_x = seepage velocity along the primary, longitudinal direction of groundwater flow (m/yr)

D_x = longitudinal dispersion coefficient (m^2/yr)

D_y = transverse dispersion coefficient perpendicular to direction of groundwater flow (m^2/yr)

k = net transformation or decay rate constant (1/yr).

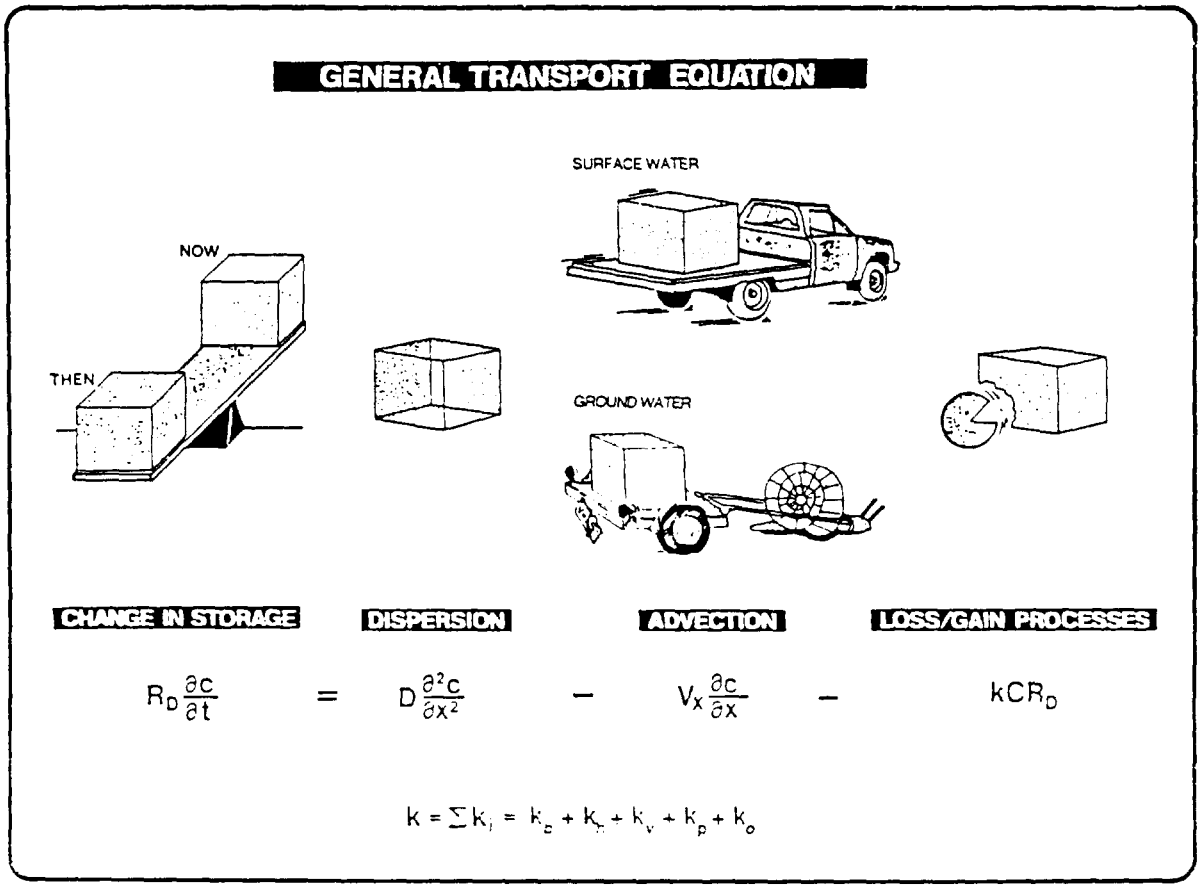


Figure 4-1. General Transport Equation. This equation in various forms, with different boundary and initial conditions, is used to describe solute transport with reaction in natural waters. Advective velocities in surface waters, e.g., rivers can be a million times larger than those (seepage velocities) in groundwater systems (e.g., compare typical velocities of about 0.5 m/sec for rivers with groundwater seepage velocities of about 10 m/yr).

The first term of the above equation represents the net rate of mass accumulation of the solute (on both liquid and solid phases), the second term represents mass flow by advection, the third and fourth terms represent mass flow by dispersion, and the last term represents net loss of mass by transformation or decay. Decay is assumed to occur at the same rate in both the liquid and solid phases. The initial background concentration in the aquifer can be equal to zero or set equal to a user-specified value.

Prior to the time when leachate reaches the groundwater and after the time when leaching has stopped, the solute concentration in the groundwater at the origin (x = 0, y = 0) is equal to the background concentration (Figure 4-2). During the period when leaching is occurring, the solute concentration in the aquifer along the downgradient edge of the source (e.g., disposal site) (x = 0, y ± W) is set equal to the concentration in the aquifer after mixing with the leachate. Beyond the upper or lower boundaries of the source (along the Y axis), the concentration in the aquifer returns to the background concentration. The above conditions are described in mathematical terms as follows:

Initial Conditions:

$$c(x,y,0) = c_{bk} \qquad 0 \le x < \infty, \quad -\infty \le y < \infty$$

Boundary Conditions:

$$c(0,y,t) = c_{bk} \text{ when } 0 \le t \le t_{on}$$

$$c(0,y,t) = c_{bk} \text{ when } y > \frac{W}{2} \text{ or } y < -\frac{W}{2};\ t_{on} \le t \le t_{off}$$

$$c(0,y,t) = c_o \text{ when } -\frac{W}{2} \le y \le \frac{W}{2};\ t_{on} < t < t_{off}$$

$$c(0,y,t) = c_{bk} \text{ when } t > t_{off}$$

$$\frac{\partial c}{\partial x}(\infty,y,t) = 0$$

$$\frac{\partial c}{\partial y}(x,\infty,t) = 0$$

$$\frac{\partial c}{\partial y}(x,-\infty,t) = 0$$

where

c_{bk} = background solute concentration in aquifer (mg/l or µg/l)

W = width of the source (e.g., disposal site) perpendicular to the direction of flow (m)

c_o = concentration in aquifer at downgradient edge of the source (e.g., disposal site) (mg/l or µg/l)

t = time (yr).

x = longitudinal distance from disposal site in primary flow direction (m)

y = transverse distance from center of disposal site perpendicular to the primary flow direction (m)

t = time (years)

t_{on} = time when leachate starts entering the groundwater (yr, e.g., 1985 or 0)

t_{off} = time when leachate ceases entering the groundwater (yr, e.g., 1988 or 3)

D_x = longitudinal dispersion coefficient (m^2/yr)

D_y = transverse dispersion coefficient (m^2/yr)

V_x = longitudinal groundwater seepage velocity (m/yr)

W = width of disposal site (m)

R_d = retardation factor for linear equilibrium sorption (dimensionless), if no sorption ($R_d = 1$)

k = net transformation or decay rate constant (1/yr)

erfc(:) = complimentary error function (dimensionless).

The above equation is solved by the code using the Gauss-Legendre quadrature integration scheme and the integral transform method.

For the 2-D cross-sectional cases, the solution is modified to take into account the finite depth of the saturated zone. The bottom of the aquifer is taken to be an impermeable boundary. This is done using the method of images (Carslaw and Jaeger, 1959). The approach is implemented by first computing solute concentrations due to the actual leachate source. Next, the problem is solved for an image source located below the bottom of the aquifer as shown in Figure 4-3. The concentration of solute which is within the aquifer is added to the original solution. The predicted values due to the image source could also cross the upper boundary of the aquifer (i.e., the water table). A second source above the aquifer is added as shown in Figure 4-4. The concentration of solute computed to be within the aquifer is again added to the original solution. This accounts for "loss" across the water table. The code keeps adding image sources (up to 11) to correct for boundary effects until the change in concentration is less than a specified tolerance. These calculations are performed automatically.

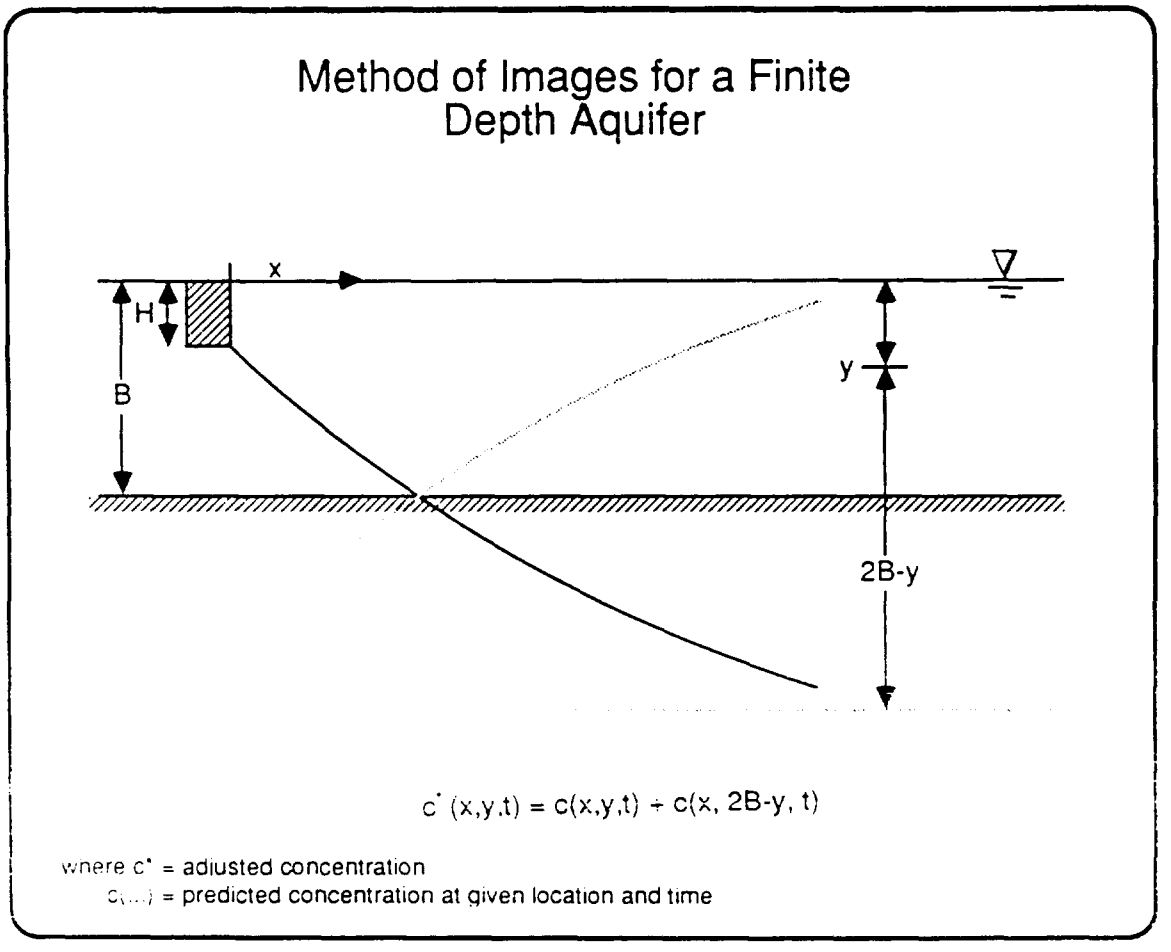
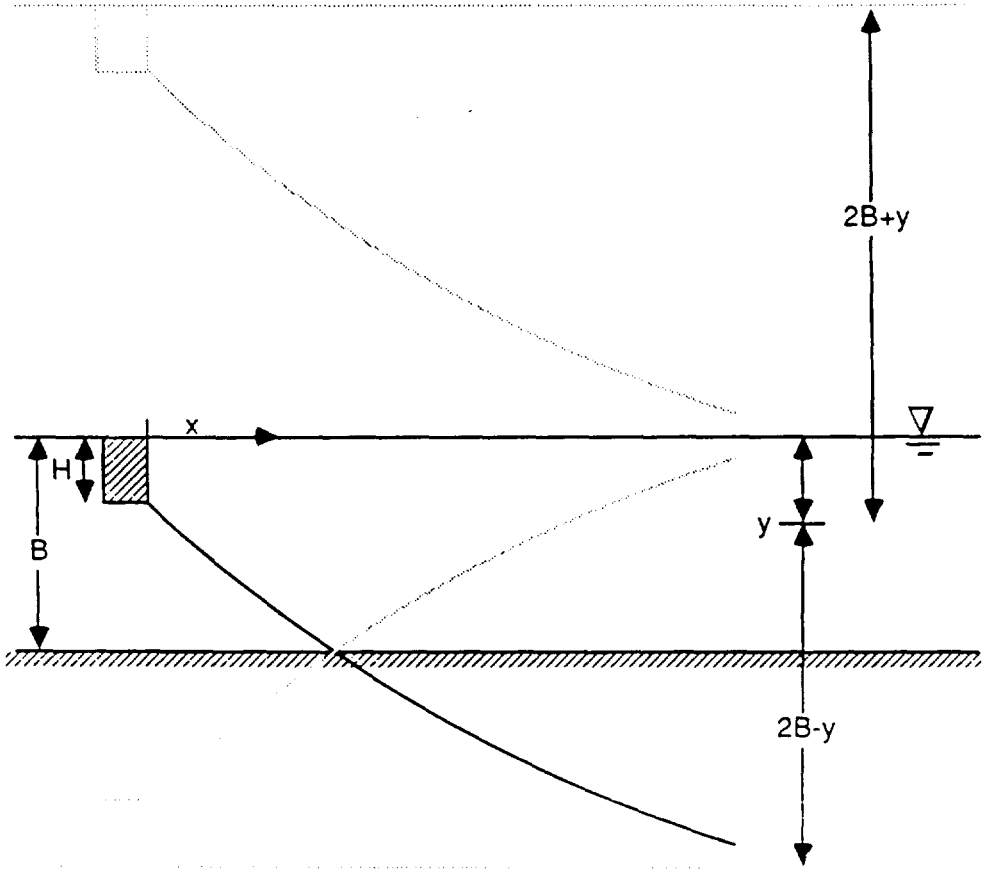


Figure 4-3. Schematic showing position of image source to correct for lower impervious aquifer boundary.



$$c^{*}(x,y,t) = c(x,y,t) + c(x, 2B-y, t) + c(x, 2B-y, t)$$
$$c(x, 4B-y, t) + c(x, 4B-y, t) + \ldots$$

where c^{*} = adjusted concentration
$c(\ldots)$ = predicted concentration at given location and time

Figure 4-4. Schematic showing addition of a second image source to correct for upper boundary of aquifer.

Governing Equation and Solution for One-dimensional Case

The partial differential equation for the 1-D case is given below:

$$R_d \frac{\partial c}{\partial t} + V_x \frac{\partial c}{\partial x} = D_x \frac{\partial^2 c}{\partial x^2} - kcR_d \qquad (4\text{-}2)$$

where:

R_d = retardation factor for linear, equilibrium sorption (dimensionless), if no sorption ($R_d = 1$)

c = concentration of solute in groundwater (mg/l or µg/l)

t = time (yr)

V_x = seepage velocity along primary, longitudinal direction of groundwater flow (m/yr)

D_x = longitudinal dispersion coefficient

k = net transformation or decay rate constant (1/yr).

The terms in the above equation are analogous to those discussed for the 2-D case. They represent the net rate of mass accumulation, mass flow by advection, mass flow by dispersion, and net transformation or decay. The initial conditions and boundary conditions are given below:

Initial Condition: $c(x,0) = c_{bk}$ when $0 \leq x < \infty$

$c(0,t) = c_{bk}$ when $0 \leq t \leq t_{on}$

Boundary Conditions: $c(o,t) = c_o$ when $t_{on} \leq t_{off}$

$c(o,t) = c_{bk}$ when $t > t_{off}$

$\frac{\partial c}{\partial x}(\infty,t) = 0$

where

c_{bk} = background solute concentration in aquifer (mg/l or µg/l)

c_o = concentration in aquifer at downgradient edge of source (e.g., disposal site) (mg/l or µg/l)

t = time (yr).

The solution to equation 4-2 is as follows (Cleary and Ungs, 1978 and Javandel et al., 1984):

a) before leachate has reached the groundwater

$$\text{for } 0 \le t \le t_{on}$$
$$c(x,t) = c_{bk}$$

b) during the time when leachate is entering the groundwater

$$\text{for } t_{on} < t \le t_{off}$$

$$c(x,t) = c_{bk} + \frac{(c_o - c_{bk})}{2}\left\{e^{-2ab} \cdot \operatorname{erfc}(-a\sqrt{t-t_{on}} + b/\sqrt{t-t_{on}}) + e^{2ab} \cdot \operatorname{erfc}(a\sqrt{t-t_{on}} + b/\sqrt{t-t_{on}})\right\} \cdot e^{V_x x/(2D_x)}$$

c) after leachate has ceased entering the groundwater

$$\text{for } t > t_{off}$$

$$c(x,t) = c_{bk} + \frac{(c_o - c_{bk})}{2}\left\{e^{-2ab} \cdot \operatorname{erfc}(-a\sqrt{t-t_{on}} + b/\sqrt{t-t_{on}}) + e^{2ab} \cdot \operatorname{erfc}(a\sqrt{t-t_{on}} - b/\sqrt{t-t_{on}})\right\} \cdot e^{V_x x/(2D_x)}$$
$$- \frac{(c_o - c_{bk})}{2}\left\{e^{-2ab} \cdot \operatorname{erfc}(-a\sqrt{t-t_{off}} + b/\sqrt{t-t_{off}}) + e^{2ab} \cdot \operatorname{erfc}(a\sqrt{t-t_{off}} + b/\sqrt{t-t_{off}})\right\} \cdot e^{V_x x/(2D_x)}$$

where

$$a = \sqrt{k + V_x^2/(4R_d D_x)} \quad ; \quad b = \sqrt{x^2 R_d/(4D_x)}$$

c_o = concentration in aquifer at downgradient edge of source (e.g., disposal site (mg/l or µg/l)

c_{bk} = initial background concentration of solute in the aquifer (mg/l or µg/l)

c = concentration of solute in aquifer at distance x and time t (mg/l or μg/l)

x = distance from disposal site in direction of primary flow (m)

t = time (yr)

t_{on} = time at which leachate enters the aquifer (yr, e.g., 1980 or 0)

t_{off} = time at which leachate from disposal site stops entering the aquifer (yr, e.g., 2000 or 20)

D_x = longitudinal dispersion coefficient (m^2/yr)

V_x = longitudinal groundwater seepage velocity (m/yr)

R_d = retardation factor for linear, equilibrium sorption (dimensionless)

k = decay rate constant (1/yr)

erfc(:) = complimentary error function (dimensionless).

The Gauss-Legendre quadrature integration scheme and the integral transform method are also used to solve the 1-D cases. The true 1-D equation is solved by the code. A modified solution is also included in the code to handle cases with very small dispersion or with no dispersion (i.e. advection only).

Assumptions

The major assumptions of the model are listed below:

- The groundwater seepage velocity remains constant over the distance of a given simulation.
- Dispersion is represented by Fick's Law. The coefficients remain constant for a given simulation.
- Sorption is treated as linear, equilibrium partitioning between aqueous and solid phases.
- Transport of a single solute species for a given simulation is adequate. Interactions between species are not considered (e.g., competition for sorption sites between sulfate and trace elements).
- First order kinetics adequately simulate solute transformation or decay. The decay rate is assumed to be the same for solutes present in either the solid or liquid phases.

The use of a constant seepage velocity, usually set equal to the average value, is a requirement for most analytical models. Except in areas with large vertical gradients

or inhomogeneous, layered systems with wide variations in hydraulic conductivity, this assumption is a reasonable approximation for screening level calculations.

Dispersion in groundwater is not well-understood and is being investigated by EPRI, EPA, USGS, and others (Gelhar et al., 1985; Molz et al., 1983; Betson, 1985; Roberts et al, 1986; LeBlanc, 1984; and Harvey, et al., 1989). To evaluate effects on predictions due to uncertainty associated with dispersivity constants, sensitivity analyses can be run using the multiple simulations option. In addition, the apparent scale dependency of dispersion can be considered by selecting specific values of dispersivity for each distance of interest. For example, a value could be selected corresponding to the distance to a monitoring well 30 m downgradient and another one for a surface water body located 300 m downgradient.

Linear partitioning is an adequate approximation for simulating equilibrium sorption of most solutes in groundwater (Figure 4-5). At high concentrations, such as may occur in interstitial solution concentrations, a linear representation may not be applicable. The retardation factor used for "metals" should be based on a partition coefficient (K_d) value which is appropriate for the pH, redox conditions, and ionic strength found in the aquifer (Rai and Zachara, 1984 and 1986). The retardation factor is assumed to be constant for a given simulation. For organics, the retardation factor can be estimated using the organic carbon content and grain-size distribution of the permeable formation. Estimation of retardation factors is discussed further in Section 5 of this report "Estimation of Input Data" and in Eary and Rai, 1988.

Because of the formulation of the code's equations, it is not appropriate for simulating storm events or for tracking a wetting front through an unsaturated formation. The code can, however, provide an estimate of transport through the unsaturated zone if one is willing to use the approximation of a constant moisture content (representing a particular set of hydrologic and meteorologic conditions beneath a disposal site). Given that wastes may leach for long periods of time (e.g., tens or even hundreds of years) and that users may be interested in the concentrations at the water table rather than the concentration profile over depth in the unsaturated zone, such approximations can be useful for screening purposes. One could run the code using a range of typical moisture content values to show the variation in concentration vs. time due to this factor.

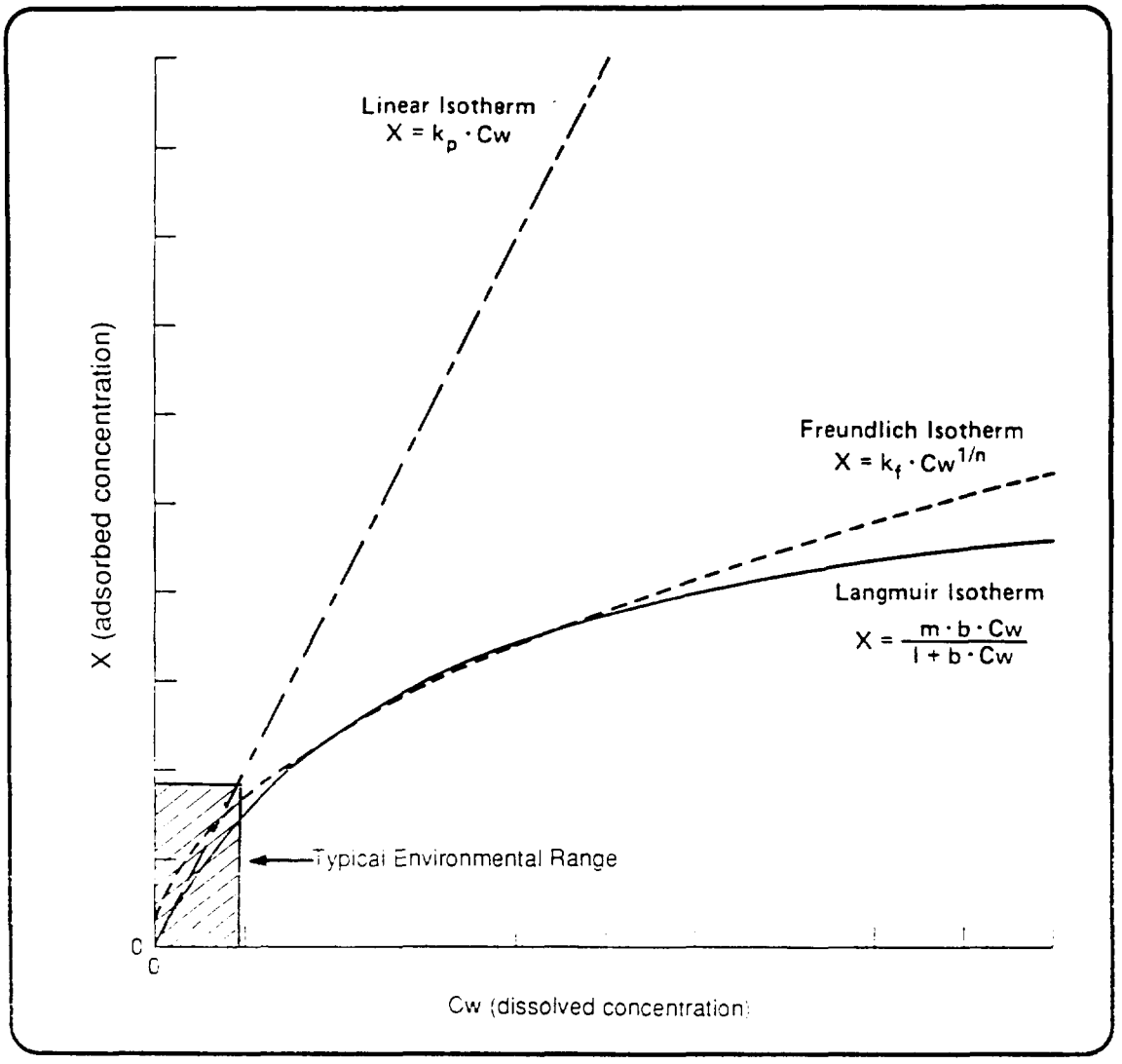


Figure 4-5. Hypothetical curves based on alternative formulations for adsorption (after Mills et al., 1985).